Structure Determination of PITP Using MAD Techniques

M.D. Yoder and L.M. Thomas (U. of Missouri-Kansas City), J.M. Tremblay (Kansas U. Medical School), R.L. Oliver (U. of Missouri-Kansas City), L.R. Yarbrough and G.M. Helmkamp, Jr. (Kansas U. Medical School)

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Introduction: The crystal structure was determined of rat phosphatidylinositol-transfer protein (PITP) complexed to one molecule of phosphatidylcholine.

Methods and Materials: A three-wavelength MAD X-ray data set was collected on beamline X12C utilizing the 'Fed-Ex Data Collection' procedures. The 271 amino acid protein contained eight Se-methionine residues.

Results: The protein crystallizes in spacegroup P21 with a=43.914 Å, b=73.773 Å, c=48.185 Å, and ß = 114.732º. There is one molecule per asymmetric unit. The x-ray data was processed by HKL to 2.2 Å, with an overall completeness of 90%. Five Se sites were determined by SOLVE and refined by SHARP. Currently the model consists of protein residues 2-270, 55 water molecules, and one molecule of phosphatidylcholine. The crystallographic R-factor is 21.2% and the free R-factor is 25.3%

Conclusions: The structure of PITP was successfully determined by x-ray diffraction analysis. Coordinates have been deposited in the Research Collaboratory for Structural Bioinformatics Protein Databank with accession code 1FVZ.

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